

Time-dependent Hartree-Fock study on photoinduced dynamics in two-dimensional organic conductors

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Photoinduced melting of charge order (CO) in quasi-two-dimensional organic conductors α -(ET)₂I₃ (ET=BEDT-TTF) and θ -(ET)₂RbZn(SCN)₄ is investigated theoretically. α -(ET)₂I₃ and θ -(ET)₂RbZn(SCN)₄ are the typical compounds with a quarter filled π -band which are known to exhibit CO. The photoinduced melting of CO in these systems has been observed by using the femtosecond spectroscopy recently[1]. It indicates that a semimacroscopic metallic domain is generated for α -(ET)₂I₃, whereas only local melting of CO is created for θ -(ET)₂RbZn(SCN)₄. In particular, the dynamics in α -(ET)₂I₃ shows critical slowing down and strong dependence on the excitation intensity and temperature. This clear difference is considered to originate from the roles of lattice distortion in stabilizing COs. In fact, the transition is of first-order with a large structural distortion and large discontinuity in θ -(ET)₂RbZn(SCN)₄, whereas the lattice distortion in α -(ET)₂I₃ is relatively small. These observations are consistent with the theoretical calculations with Hartree-Fock approximation[2,3]. Therefore, it is of great interest to investigate the photoinduced melting of CO in these systems and compare their dynamics.

In order to study the photoinduced dynamics in each compound, we solve the time-dependent Schrödinger equation numerically within the Hartree-Fock approximation for an extended Peierls-Hubbard model. The obtained charge, spin and lattice dynamics are considered to reflect the different natures of charge ordered states in these systems. In particular, the melting of CO needs more energy for θ -(ET)₂RbZn(SCN)₄ than for α -(ET)₂I₃, which is a consequence of large lattice distortion and the essential role of electron-phonon coupling in stabilizing the CO in θ -(ET)₂RbZn(SCN)₄.

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